Electronic Supplementary Information

Encapsulation of divalent tetrahedral oxyanions of sulfur within rigidified dimeric capsular assembly of tripodal receptor: First crystallographic evidence of thiosulfate encapsulation

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Fig. S1 $^1$H NMR spectrum of receptor L in DMSO-$d_6$ at 298K.
Fig. S2 $^{13}$C NMR spectrum of receptor L in DMSO-$d_6$ at 298K.
Fig. S3 ESI Mass spectrum of L.
Fig. S4 NOESY spectrum of L.
Fig. S5 IR spectrum of receptor L.

Fig. S6 Stack plot of the \(^1\)H NMR spectra of receptor L in the presence of increasing amounts of \([n-\text{Bu}4\text{N}^+]_2\text{SO}_4^{2-}\) recorded in DMSO-\(d_6\) at 298 K.
**Fig. S7** Job’s plot for L with $[n$–Bu$4N^+]_2$SO$_4^{2-}$ in DMSO-$d_6$ at 298K.

**Fig. S8** IR Spectrum of the complex 1.
Fig. S9 NOESY spectrum of L in presence of one equivalent SO$_4^{2-}$ anion.
Fig. S10 Stack plot of the $^1$H NMR spectra of receptor L in the presence of increasing amounts of Na$_2$S$_2$O$_3$ recorded in DMSO-$d_6$ at 298 K.

Fig. S11 IR Spectrum of the complex 2.
Fig. S12 NOESY spectrum of L in presence of one equivalent S$_2$O$_3^{2-}$ anion recorded in DMSO-$d_6$ at 298 K.
**Fig. S13** Powder X-ray diffraction: simulated pattern from the single-crystal X-ray of complex 1 (black), experimental pattern from the crystalline solid obtained in presence of sulfate anion (red), experimental pattern from the crystalline solid obtained in presence of hydrogensulfate anion (blue).

**Fig. S14** Powder X-ray diffraction: simulated pattern from the single-crystal X-ray of complex 2 (black), experimental pattern from the crystalline solid of complex 2 (red),
**Fig. S15** $^1$H NMR spectrum of complex 1 recorded in DMSO-$d_6$ at 298 K.
**Fig. S16** $^{13}$C NMR spectrum of complex 1 recorded in DMSO-$d_6$ at 298 K.
Fig. S17 $^1$H NMR spectrum of complex 2 recorded in DMSO-$d_6$ at 298 K.
Fig. S18 $^{13}$C NMR spectrum of complex 2 recorded in DMSO-$d_6$ at 298 K.
Fig. S19 Depicting sulphate encapsulated receptor segment is present in the hydrophobic pocket of TBA counter cations in complex 1.